Influence of Ions on the Coalescence Behavior

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Introduction

Continuous settlers are used in many processes for separating liquid-liquid dispersions. In a efficient process, this downstream operation must be sufficiently well designed so that the dispersion is completely split into two separate phases.

However, trace components influence the coalescence and thus the settling behavior. It varies with the ions type and with their concentration making settling quite unpredictable. Usually, settling experiments are conducted in a so-called settling cell. From the experiment, the system can be characterized [1,2].

A numerical tool, based on the ReDrop concept (Representative Drops) [1], was developed in order to simulate the separation of liquid-liquid dispersion and thus to improve the design of continuous settler. Sedimentation and coalescence are evaluated for a sufficiently large ensemble of representative individual drops at each time step.

The coalescence modeling is a major challenge in these simulations due to trace components influence and is investigated in detail.

ReDrop concept

definition of the system
- material properties:
  density, viscosity, etc.
- simulation parameters:
  initial hold up, drop-size distribution, time step, coalescence parameter, etc.

time loop
local holdup evaluated for each height element

drop loop
- individual velocity via sedimentation model
- vertical position of each drop
- Monte Carlo approach to evaluate the coalescence frequency between drops

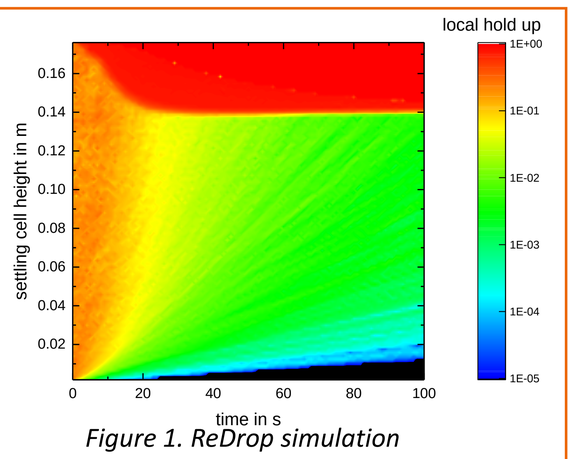

Figure 1. ReDrop simulation

- horizontal position of drops is assumed to be randomly distributed, special care is taken to evaluate contact probability to quantify correctly the coalescence
- the initial drop-size distribution can be defined as experimentally determined with the SOPAT probe
- gas bubbles and solid particles can be accounted for as additional dispersed phases

Coalescence model

- fluid-dynamic dependent variables have to be characterized once for a dedicated equipment
- the coalescence time depends on the material properties: solvent, salt concentration, trace components

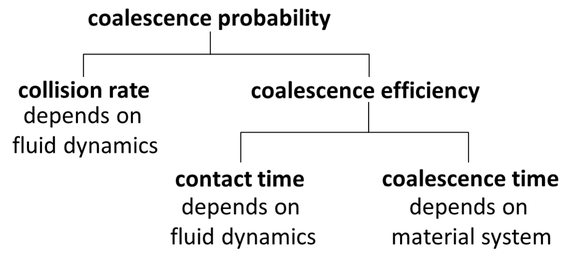

Figure 2. The coalescence model [3]

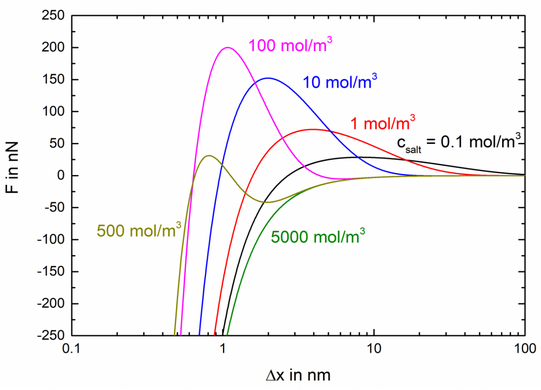

Figure 3. Typical evolution of the DLVO force with the distance between two drops [4]

- DLVO theory describes the force resulting from the repulsive ionic and the van-der-Waals forces acting between two approaching drops
- DLVO theory can be used to explain the salt influence on the coalescence [4]
- for the salt concentration, which induces a maximum force, the repulsive force between drops is large and hinders the coalescence [4]
- DLVO force related to the coalescence time

Material and Method

- system paraffin oil + deionized water with salt is chosen in order to play easily with the viscosity
- different paraffin oil viscosity and salt concentration are tested
- ReDrop simulation will be compared to the settling experiments in order to validate the coalescence model

Table 1. Density and viscosity of a specific studied system

		25°C
saturated paraffin oil	density (kg/m³) viscosity (mPas)	819.597 8.48
saturated deionized water + 50 mmol/L of NaCl	density (kg/m³) viscosity (mPas)	999.041 1.030

- the two-phase system is stirred during 30 sec at 800 min^{-1}
- experiments are conducted 3 times to validate reproducibility
- the settling time is reached when only half of the interface remains covered by a monolayer of droplets
- experiments are recorded on video in order to obtain the experimental data point
- SOPAT inline probe is used to measure the initial drop-size distribution

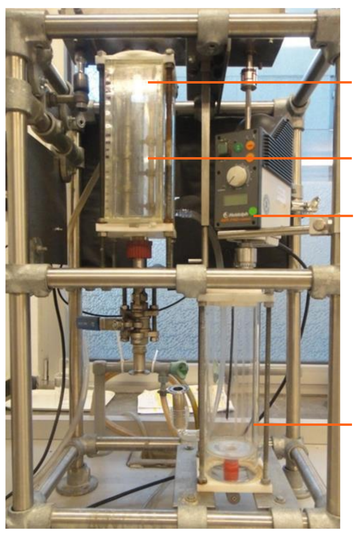

Figure 4. Henschke settling cell

First results

ReDrop modelling

Different phenomena have been taken into account through models in order to simulate their effect on the settling:
- the drops velocity
- the coalescence probability in the close-packed and the sedimentation zone
- the collision frequency in the sedimentation zone to evaluate the coalescence probability between two meeting drops. [7]
- the contact time between two meeting drops. Motion simulation of the two drops has been compared to literature. [6]
- the hydrostatic pressure in the close-packed zone, which has an effect on the drop deformation and the coalescence efficiency. It depends on the height of the buoyant drops and on the counter flow of the liquid phase around the drops.
- the dodecahedron deformation of the drops in the close-packed zone. [1] It varies with the hydrostatic pressure and it has an effect on the local hold up
- the random global packing of drops in the close-packed zone has been studied as well

ReDrop simulation

- the developed coalescence model was applied together with the SOPAT measurements in order to describe the settling behavior as shown in Fig. 6.
- curved sedimentation profile and remaining drops are observed during the experiment and simulated with the ReDrop program

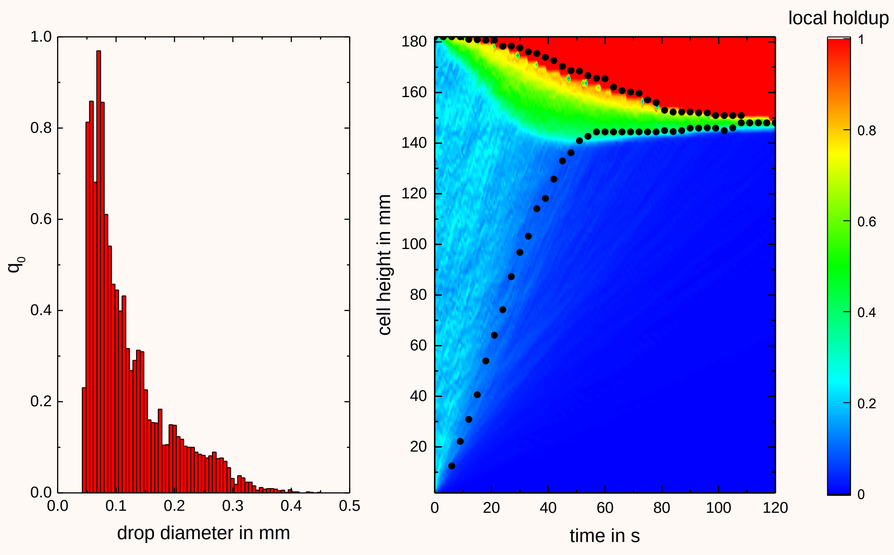

Figure 6. Simulation of settling experiment with the ReDrop tool.

Conclusion

The simulation of settling experiments with the ReDrop program is in good agreement with observations. As next steps, further investigations will include the DLVO theory in the coalescence model.

References
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